Regularization by Control of the Resolution Function

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Abstract
Unfolding based on Singular Value Decomposition is used to illustrate how regularization is related to control of the resolution function and thereby the interpretation of the unfolding result.

1 Introduction

A central problem in many data analyses is the correction of the raw measurements for distortions caused by the experimental setup. In the 1-dimensional case the mapping between a true physical density $b(y)$ and the experimentally observable one $a(x)$ is given by the integral equation

$$a(x) = \int dy \; g(x,y) \cdot b(y) \; . \tag{1}$$

In the high energy physics use case the unknown $b(y)$ often is proportional to a cross-section, i.e. non negative. In the following the response function $g(x,y)$, which for a given true value y is the probability density function for the actually observed quantity x, is assumed to be known. In typical applications the observable density $a(x)$ is estimated in a counting experiment. Since a finite number of events cannot fully determine a continuous function $a(x)$, it is obvious that some discretization has to be performed. A widely used and intuitive way to discretize density functions is by means of histograms, i.e. average densities over finite intervals rather than truly continuous functions. Equation (1) then becomes

$$a_k = \sum_{i=1}^{n} G_{ki} \cdot b_i \qquad \text{with} \qquad k = 1, 2, \ldots m \tag{2}$$

where a_k and b_i are the integrals over finite bins in x and y, respectively. The response function $g(x,y)$ translates into the response matrix G_{ki}. It is worth noting that for finite bin widths Δy the response matrix will general still depend on the unknown $b(y)$. Only in the limit of infinitesimal bin sizes the modeling of the detector response becomes truly independent of $b(y)$. In the following these kind of discretization errors will be ignored.

Before going further it is instructive to analyze the structure of the problem in terms of Fourier analysis [1]. Introducing an amplitude function $A(\omega)$ for the true distribution $b(y)$ and assuming a Gaussian response function $g(x,y)$ one schematically finds

$$b(y) = \int d\omega \; A(\omega) \cos(\omega y) \tag{3}$$

and

$$a(x) = \int dy \; \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-y)^2/2\sigma^2} \cdot b(y) = \int d\omega \; e^{-\omega^2\sigma^2} \cdot A(\omega) \cos(\omega x) \; . \tag{4}$$

The high frequency components of the observable density $a(x)$ are exponentially suppressed by the finite resolution σ of the response function, and thus can only be measured in the limit of very high statistics. It follows [2] that in practice unfolding will not be able to perform a complete correction but should rather be understood as "improvement of the resolution function". This shall be made more quantitative in the following.

2 Singular Value Decomposition

Singular Value Decomposition (SVD) highlights the properties of any matrix $Q[m, n]$ with m rows and n columns and $m \geq n$ by factorizing it in the form

$$Q[m, n] = U[m, n] \cdot W[n, n] \cdot V[n, n]^T \tag{5}$$

with a non-negative diagonal matrix W and orthogonal matrices U and V satisfying

$$U^T \cdot U = V^T \cdot V = V \cdot V^T = \mathbf{1}_n \,. \tag{6}$$

Here $\mathbf{1}_n$ denotes the unit matrix in n-dimensions. The diagonal elements of W are the "singular values" of Q, usually sorted in descending order.

SVD allows to analyze the nature of a given unfolding problem by diagonalizing it [3]. The first step is a linear transformation M of the measurements a to $a' = M\,a$ such that the covariance matrix of a' becomes the unit matrix, $C(a') = M\,C(a)\,M^T = \mathbf{1}_m$. SVD of the transformed unfolding problem then yields

$$a' = (M\,G)\,b = (U\,W\,V^T)\,b \tag{7}$$

and, introducing *normalized measurements* $u = U^T a'$ with again unit covariance matrix $C(u) = U^T\,C(a')\,U = \mathbf{1}_n$, the diagonalized unfolding problem can be expressed in the form

$$u = W\,V^T\,b \qquad \text{or} \qquad W^{-1}\,u = V^T\,b\,. \tag{8}$$

The first equation in eq.(8) is a discrete analog of eq.(4) for an arbitrary response matrix. The vector u is a representation of the measurements where the individual components are uncorrelated and have unit variance, and $V^T\,b$ the expansion of the discretized true distribution into the orthonormal basis provided by the rows of V^T. The connection between the two is given by the diagonal elements of W, which for typical problems has a steeply falling spectrum of singular values. The higher order expansion coefficients of b thus quickly reach expected values close to zero, which the measurements with unit errors cannot resolve.

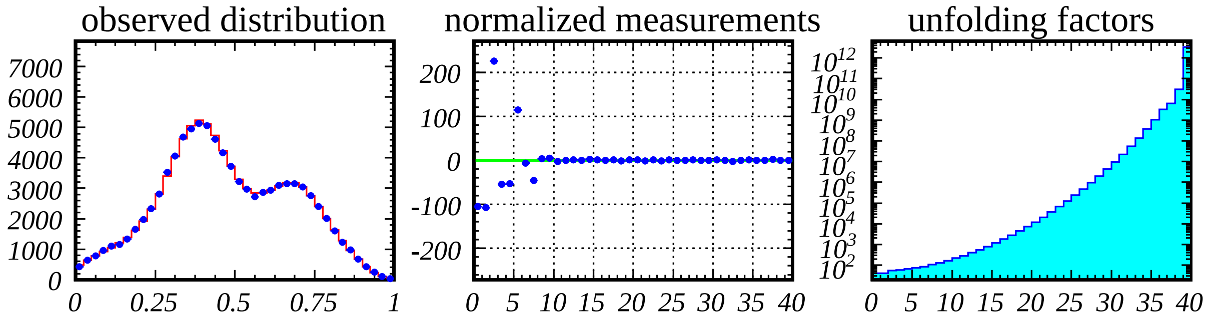

Fig. 1: Observed distribution with 10^5 events compared to the expectation (left), normalized measurements (center) and unfolding factors, i.e. the inverse of the singular values of the diagonalized unfolding problem (right).

This is illustrated by an example [1] with a true distribution $b(y)$ defined on the interval $y \in [0, 1]$ and response function $g(x, y)$

$$\begin{aligned} b(y) &= \frac{20.334}{100 + (10y-2)^2} + \frac{2.0334}{1 + (10y-4)^2} + \frac{4.0668}{4 + (20y-15)^2} \\ g(x, y) &= \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(x - \left[y - \frac{1}{10}y^2\right]\right)^2\right) \cdot \left(1 - 2\left(y - \frac{1}{2}\right)^2\right)\,, \end{aligned} \tag{9}$$

the latter featuring a Gaussian resolution $\sigma = 0.05$, a quadratic bias, and a parabolic efficiency loss towards the phase space limit. The result of a discretization with 40 bins for the true and the observed distribution, assuming a total of 10^5 events in the measured distribution is shown in Fig. 1. One clearly sees that under the assumed conditions only the leading 10 to 15 coefficients of the solution are experimentally accessible. Using higher order coefficients to reconstruct the unfolded distribution will mainly amplify statistical fluctuations. So only the leading order coefficients of the expansion of the solution can be determined experimentally.

Not knowing the higher order coefficients implies that the fine structure cannot be fully resolved. There is a loss of resolution, and the question arises whether it is possible to quote some equivalent Gaussian resolution.

This can be answered heuristically by studying the expansion of a delta-pulse into a set of orthogonal functions. In the discrete case one simply has vector a b with components $b_i = \delta_{iI}$, i.e. zero everywhere except for component I, which is expanded into an orthogonal basis $v_k, k = 1, \ldots, n$. Such a basis is, for example, given by the columns of the matrix V introduced above. The expansion coefficients u_k are obtained by the scalar products $u_k = v_k \cdot b = v_{kI}$. Zeroing (i.e. discarding) the higher order coefficients in order to study what happens when those are not known, and re-synthesizing the content of bin I then yields

$$\hat{b}_I = \sum_{k=1}^{j} u_k \, v_{kI} = \sum_{k=1}^{j} v_{kI}^2 \ . \tag{10}$$

For $j = n$, i.e. in case all expansion coefficients are used, one recovers $\hat{b}_I = b_I = 1$. The truncated sum has $\hat{b}_I < 1$, but non-zero content in the neighboring bins.

The same happens when a delta-function is smeared by a Gaussian. The integral over the central bin is no longer unity, and part of the normalization ends up in the neighboring bins. This suggests to define an equivalent Gaussian resolution σ by the condition

$$\int_{-w/2}^{w/2} dx \, \frac{1}{\sqrt{2\pi}\sigma} \, e^{-x^2/\sigma^2} = \hat{b}_I \ , \tag{11}$$

with w the bin width and the parameter σ chosen such that the central bin has the same content as that of the truncated re-synthesis. One finds

$$\frac{\sigma}{w} = \frac{1}{\sqrt{8}\,\mathrm{erf}^{-1}(\hat{b}_I)} \oplus \frac{1}{\sqrt{12}} \ . \tag{12}$$

The term $1/\sqrt{12}$ (to be added in quadrature) has been put by hand to account for the fact that even for $b_I = 1$ the attainable resolution is limited by the finite bin width. Figure 2 shows for the above example that this heuristic approach gives a realistic estimate for the actual resolution of the truncated series.

3 Unfolding

The above example shows that only the leading order coefficients of the expansion of the solution into an orthonormal basis can be used for the construction of the unfolded distribution. Nevertheless, the resolution of the truncated result will usually be better than the resolution of the measurement. Also, biases and efficiency losses will be corrected.

Suppression or, more generally, adjustment of the insignificant components is also referred to as "regularization". The simplest scheme is to fix them to zero. Alternative choices, for example asking for minimal curvature or Maximum Entropy of the unfolding result can be employed to supply the missing coefficients. In general everything is allowed which is consistent with the measurements, including adjusting the well measured leading order coefficients within their uncertainties. In all cases the resolution of the result is determined by the number of coefficients which are used.

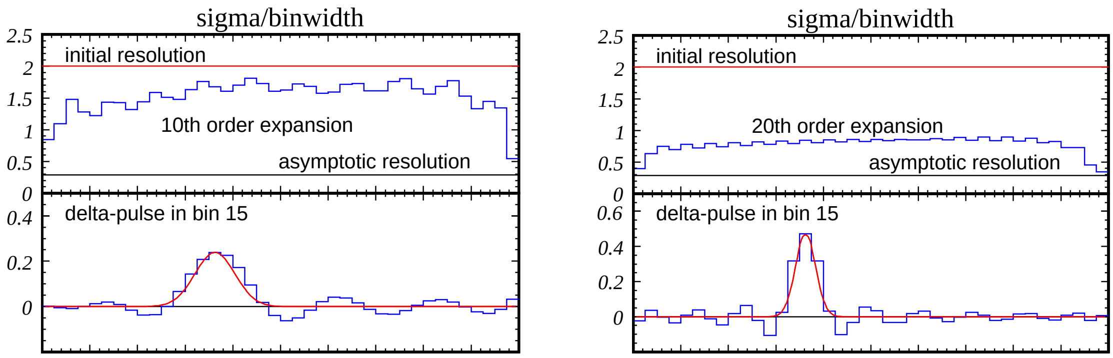

Fig. 2: Resolution of a truncated expansion into an orthogonal basis using the leading 10 (left) or 20 (right) from a total of 40 expansion coefficients. The actual values apply for the example discussed in the text. The resolution is given in units of the bin width, i.e. the asymptotic value is $1/\sqrt{12}$. The initial resolution of $\sigma = 0.05$ corresponds to the width of 2 bins. In the top parts the estimated resolution is shown as a function of the bin number, the lower parts compare the Gaussian estimates (continuous line) with the truncated synthesis (histogram) for a delta-pulse in bin 15.

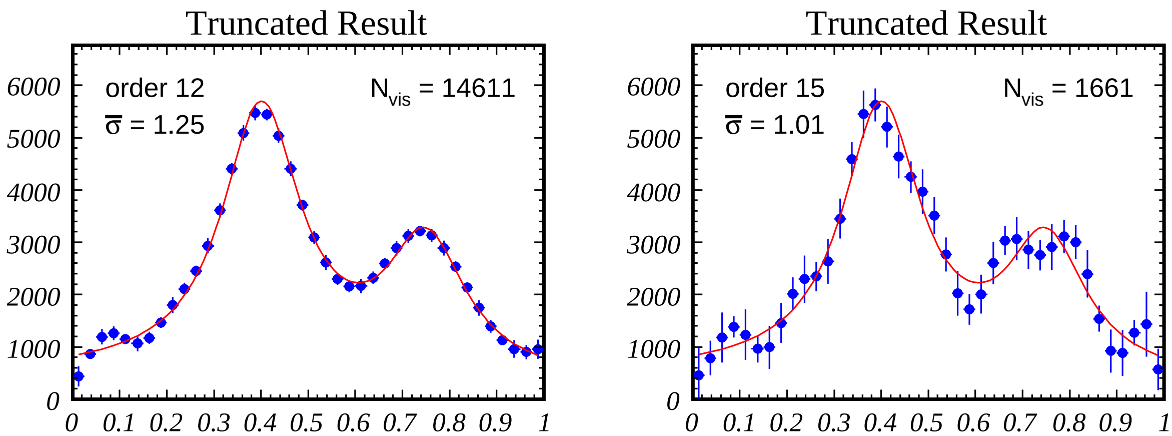

Fig. 3: Unfolding results based on the leading 12 (left) or 15 (right) coefficients of the expansion of the solution into an orthonormal basis. Also shown (continuous line) is the true distribution for the problem studied. Comparing the two results illustrates how better resolution (smaller $\bar{\sigma}$) implies larger uncertainties.

Figure 3 shows the unfolded distribution for the example introduced above when using either the leading 12 or the leading 15 coefficients. The errors are obtained by linear error propagation. Two figures-of-merit to judge the result are given, the average resolution $\bar{\sigma}$ in units of the bin width, obtained by averaging eq.(12) over all bins, and the visible statistics in the unfolded histogram defined as $N_{\text{vis}} = (\sum b_i)^2 / \sum \sigma^2(b_i)$. The quantity N_{vis} is constructed such, that for independent poissonian errors it is identical to the number of entries in the histogram. While $\bar{\sigma}$ is proportional to correlation length between neighboring bins, N_{vis} is a simple measure for the smoothness of the result. For any quantitative statements regarding errors the full covariance matrix of the result has to be considered.

In both cases the unfolding result is consistent with the true distribution, which is overlayed in the plots. The bias and efficiency losses assumed in the model are corrected, and the resolution which initially was $\sigma/w = 2$ is improved to $\bar{\sigma} = 1.25$ and $\bar{\sigma} = 1.01$, respectively, Since the true distribution is sufficiently smooth, already the low order result looks good. The bins of the unfolded distribution, however, are correlated. When interpreting the result, one has to be aware that statements about average densities can only be made for regions like the FWHM of the effective resolution. To make this explicit the final results should be rebinned accordingly, taking into account the correlations between the bins.

4 Conclusions

Unfolding in general can only partly correct for distortions caused by an imperfect detector in the sense that the result still is a limited resolution image of the actual truth. This partial correction is referred to as regularization. For sufficiently smooth distributions it will render the unfolding result indistinguishable from the truth. The level of regularization can be characterized by the resolution of the unfolding result, which indicates the typical range over which reliable density estimates can be obtained. In this paper regularization was performed by a simple SVD-based truncation of insignificant components. More sophisticated methods, using also a priori information like positivity will in general perform better. Nevertheless, the basic features caused by information loss due to finite resolution are universal.

References

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[3] A. Höcker and V. Kartvelishvili, "SVD Aproach to Data Unfolding", NIM A 372 (1996) 469.